Industrial Technologies Program

Enhanced Productivity Of Chemical Processes Using Dense Fluidized Beds

Enabling Computational Technology Will Directly Impact the Energy Requirements of Catalytic and Non-Catalytic Reaction Processes

Throughout the chemical industry, dense gas-solid reactors such as fluidized beds are used for catalytic and non-catalytic reaction processes. However, understanding, control, and scale-up of dense gas-solid reactors and fluidized beds are limited by difficulties in measuring and modeling dense multiphase flows, which are inherent to both processes. There is a large potential for energy and emission savings through further understanding of dense gas-solid flows in fluid beds that could in turn improve the production of both catalytic and non-catalytic reaction processes.

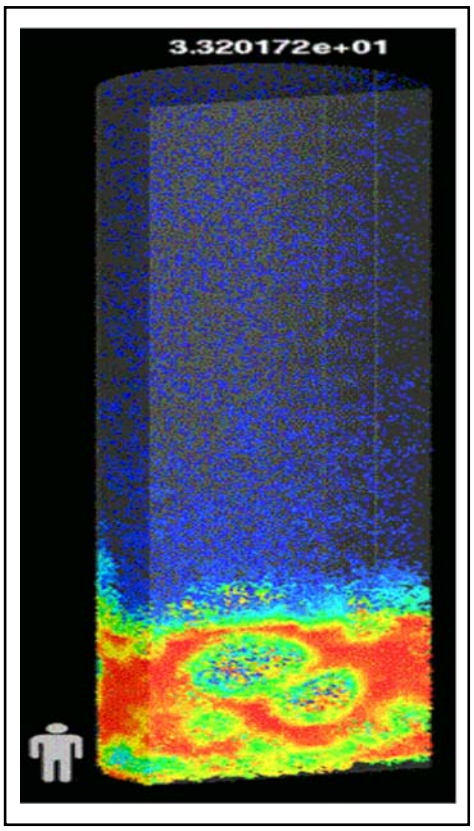

Fig. 1: Computed behavior of a large-scale fluidized bed

Millennium Inorganic Chemicals, Inc. (MCH), Arena-flow, LLC, ExxonMobil Research and Engineering Co., and Sandia National Laboratories, are working together to develop technologies that will help better predict and control the behavior of dense gas-solid reactors and fluidized beds, with the end goal of implementing these technologies at industrial plants. Potential energy savings from modeling improvements of these processes can be as high as 33 trillion Btu per year by 2020. The computational technology under investigation is cross-cutting and can be broadly applicable and commercially available to many other chemical and petroleum industry unit operations, directly enhancing facility operations throughout the industry.

Benefits

By 2020:

- *Energy savings of 33 trillion Btu per year for the U.S. chemical industry*
- *Annual energy savings of 8 trillion Btu from improvements in the Fluid and Flexicoking process*

Applications

Improvements in dense gas-solid reactor and fluidized bed modeling will yield significant energy savings across the chemical industry. Dense gas-solid reactors are used in hydrocarbon cracking, Fischer-Tropsch synthesis, and the production of titanium dioxide, polyethylene, and many other chemicals. Similarly, fluidized beds are used for chlorination, oxidation, roasting, calcinations, combustion, incineration, heat treatment, coatings, and many other processes.

Project Partners

- *Millennium Inorganic Chemicals, Inc.*
- *ExxonMobil Research and Engineering Co.*
- *Arena-flow, LLC*
- *Sandia National Laboratories*

Project Description

Goal: The overall goal of this project is to achieve significant energy savings and environmental improvements through Enabling Computational Technology.

Activities: Researchers will identify dense-bed process behaviors that ultimately limit energy savings, seek to better understand the underlying physics of particle-fluid phenomena, and develop particle-level constitutive models for basic physics and chemistry.

Work will focus on enhancing existing Arena-flow™ computational technology with new constitutive models for controlling physics of particle momentum, heat transfer, and chemistry; validating enhanced computational fluid dynamics (CFD) software against new data; and applying the technology to MCH's reactors and ExxonMobil's coking reactors.

Key project elements include the development of improved computational tools for reactor design and operation that will be implemented in a commercial computational fluid dynamics package (Arena-flow™), pilot-scale experimentation for model validation and process optimization, and commercial demonstrations of process improvements.

Progress and Milestones

Year 1 Milestones:

- Define fundamental process variables
- Identify the constitutive and numerical modeling approach
- Establish operation of pilot-scale fluidized bed experiment

Year 2 Milestones:

- Compile initial data sets from pilot-scale experiments
- Determine comprehensive pilot-scale data set
- Enhance existing capability of Arena-flow™ with the new constitutive models from the experimental task
- Validate constitutive models

Year 3 Milestones:

- Implement advanced diagnostics on industrial pilot-plant
- Validate enhanced Arena-flow™ CFD computational technology against production reactor data
- Prepare final report documenting validated computation tools
- Release the Arena-flow™ software package commercially
- Provide documentation of the dense-bed constitutive models and validations; provide training, manual, and user support
- Publish methodology demonstrating how to apply the computational technology to obtain energy enhancements

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